

Ab-initio calculations for the structural properties of $Zr - x\%Nb$ alloys

Vasyl O. Kharchenko*

*Institute of Applied Physics, National Academy of Sciences of Ukraine,
58 Petropavlovskaya St., 40030 Sumy, Ukraine and*

Institute of Physics, University of Augsburg, Universität Str. 1, D-86135 Augsburg, Germany

Dmitrii O. Kharchenko†

Institute of Applied Physics, National Academy of Sciences of Ukraine, 58 Petropavlivska St., 40030 Sumy, Ukraine

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Ab-initio calculations for the structural properties of $Zr - Nb$ alloys at different values of the niobium concentration are done at zero temperature. Cases of BCC and HCP structures are considered. Optimal values of the lattice constant together with structural relation c/a for the HCP crystals are obtained. Critical value for the niobium concentration which corresponds to the structural transformation $HCP \rightarrow BCC$ at zero temperature in alloys $Zr - Nb$ is defined. Densities of states for two different structures with niobium concentrations 12.5% and 25% which have HCP and BCC structures, accordingly, are studied.

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I. INTRODUCTION

Investigation of Zirconium alloy properties is an actual task during last 60-80 years in Nuclear Physics and Power Engineering and has very special practical significance. It is due to Zirconium and Zirconium-Niobium alloys are widely use in nuclear power industry as materials for the fuel elements, fuel assemblies and other constructions of nuclear reactors [1–3]. It is known, that Zirconium has two configurations: α -phase, which is characterize by the Hexagon Close Package (HCP) lattice and stable at not too high temperature ($< 863^\circ C$), and β -phase with Body Centered Cubic (BCC) lattice at high temperature. Niobium has BCC lattice. Zirconium-Niobium alloys which characterize by α -phase are used as construction material of the active zone of nuclear reactors because of successful a mix of nuclear, mechanical and corrosive properties [1–3].

Alloys $Zr - xNb$ with a high percentage of Niobium ($x > 5\%$) have a high capacity for hydrogenation, resulting in deterioration of corrosion properties. That is why for the reactor metallurgy Zirconium-Niobium alloys with small Niobium concentration ($< 5\%$) are useful. It is because in the nuclear reactor Hydrogen diffuses inside an alloy due to corrosion processes. When the Hydrogen concentration becomes more than solubility limit, it stands out as a fragile hydride phase, that limits the usage of an alloy in the reactor. Hence, the study of $Zr - Nb$ alloys with small and high Niobium concentration, together with processes of hydride formation in Zirconium-Niobium alloys is an actual task. Investigation of the hydride phase formation processes in alloy $Zr - Nb$ that contains 20% and 40% of Niobium was

made in [3, 4]. To study such process in alloys with high Niobium concentration the plane strain theory was used [5]. In [6] diffusion coefficients of Zr and Nb atoms in BCC alloys with Niobium concentration 5.5%, 16.3% and 28.1% were studied. It was found, that Zirconium and Niobium atoms diffuse in alloy according to the mono-vacancy mechanism. The last is defined by the specification of lattice dynamics. Diffusion of Hafnium and Niobium atoms in coarse-grained BCC alloy $Zr - Nb$ with 19% Niobium was studied in [7]. It was defined, that diffusion coefficient of Niobium is less the Hafnium one. Corrosion behavior of alloy $Zr - Nb$ with Niobium concentration variation from 0.02% to 20% was considered in [8]. It was shown, that corrosion rate becomes smaller with decrease in both bulk of the β -phase and Niobium concentration in α -phase. Authors defined that the most important factor that reduces corrosion rate is the precipitate of the $\beta - Nb$ particles and the corresponding decreasing of Niobium in the Zirconium matrix. Experimental investigations of β -phase formation with Niobium concentration 20÷88% at irradiation were made in [9–13]. Experimental results for the structural properties α - and β -phases in $Zr - Nb$ alloys with varying in Niobium concentration at high temperature ($\sim 700K$) are presented in [14–16]. Structural properties of $Zr - 12.5\%Nb$ were theoretically considered in [17]. However, the question about the critical value of Niobium concentration when the transition from α -phase toward β -phase (structural transformation $HCP \rightarrow BCC$) in Zirconium-Niobium alloys is still open.

In this work we aim to study structural properties of Zirconium-Niobium alloys with different Niobium concentration at low (zero) temperature from the first principles. Model structures of $Zr - Nb$ alloys with BCC and HCP lattices will be considered. The main task of this article is to define optimal lattice constants and in the case of HCP structures, optimal structural relation c/a for different Niobium concentration in the alloy. We shall de-

*Electronic address: vasiliiy@ipfcentr.sumy.ua

†Electronic address: dikh@ipfcentr.sumy.ua

fine the critical value of Niobium concentration that corresponds to the structural transformation HCP \rightarrow BCC at low (zero) temperature. The quantitative comparison with known experimental data will be done.

The work is organized in the following manner. In Section 2 we present models for studied structures of $Zr-Nb$ alloys and research methods description. In Section 3 we discuss structural properties and obtain optimal lattice parameters for studied structures. Analysis of total energy and density of states is done in Section 4. We conclude in the last Section.

II. MODELS OF THE STUDYING STRUCTURES AND RESEARCH METHODS

It is known, that Zirconium at low temperatures ($< 863^\circ C$) is characterized by β -phase (HCP structure), whereas Niobium has BCC structure. Hence it is naturally to expect, that alloys $Zr - xNb$ will have HCP structure at low Niobium concentration x whereas BCC structure will be stable for large x . As far as Zirconium and Niobium are different only for one electron and are characterized by close package structures one can expect that Niobium atoms in the HCP Zirconium lattice, or Zirconium atoms in the BCC Niobium lattice are substitutional atoms. In Ref.[18] authors have studied supercell of 48 atoms of HCP Zirconium which has a vacancy and Niobium atom in interstitial position placed near the vacancy. It was shown, that during relaxation processes Niobium atom takes a vacancy position. The last confirms that atoms of Zr or Nb in $Zr - Nb$ alloys are substitutional atoms.

In this article we will consider alloys $Zr - xNb$ with BCC and HCP lattices, where the Niobium concentration x takes values $x = 3.125\%$, 6.25% , 12.5% , 25.0% , 50.0% and $x = 75.0\%$ for both types of lattices, and additionally $x = 87.5\%$, 93.75% and $x = 96.875\%$ for BCC alloys. In such a case, structures with Niobium concentration 3.125% and 96.875% are characterized by the largest number of atoms in the unit cell, 32. Hence, for the given values of the Niobium concentration x in the alloy $Zr - xNb$ with the unit cell of 32 atoms, a number of Niobium atoms can be : 1, 2, 4, 8, 16, 24, 28, 30 and 31, respectively.

Model structures of BCC alloys with 2, 16 and 30 Niobium atoms in the unit cell of 32 atoms are characterized by the 221 symmetry space group; others structures have the 123 group of symmetry. All being studied structures of $Zr - Nb$ alloys with HCP lattice are characterized by the 187 space group. The number of nonequivalent atoms of Zirconium and Niobium, that gives a number of symmetry operations for each model of BCC and HCP structure is shown in Table II.

All calculations of structural and electronic properties for the model alloys, shown in table II were done in the framework of density functional theory (DFT) [19] by using linearized augmented plane wave (LAPW) method,

$\#Nb_{UC}$	Type of the lattice	$\#NEA_{Zr}$	$\#NEA_{Nb}$
1	BCC	8	1
	HCP	9	1
2	BCC	4	1
	HCP	5	1
4	BCC	3	1
	HCP	3	1
8	BCC	2	1
	HCP	2	2
16	BCC	1	1
	HCP	2	2
24	BCC	1	2
	HCP	2	2
28	BCC	1	3
	HCP	1	3
30	BCC	1	4
31	BCC	1	8

TABLE I: The number of Niobium atoms in the unit cell of 32 atoms ($\#Nb_{UC}$) and numbers of nonequivalent atoms of Zirconium ($\#NEA_{Zr}$) and Niobium ($\#NEA_{Nb}$) for each model structure with BCC and HCP lattices.

which is implemented in software packages Wien2k [20]. This method self-consistently includes basic and valence electrons and is widely used for the calculations of the band structure of solids [20].

The Muffin-tin radii (R_{MT}) of both Zr and Nb were taken to be 2.1 atomic units for all calculations. The basis function was expand up to $R_{MT} \times k_{max} = 7$, where R_{MT} is the smallest radius of the muffin-tin (MT) spheres and k_{max} is the maximal value of the reciprocal lattice vectors. Wave function expansion inside the atomic spheres was done until $l_{max} = 10$. Integration over the Brillouin zone was performed by using 1000 k -points. The criterion to stop the iteration process was converge for the total energy and charge of the crystal to less than $0.0001 Ryd$ and $0.001 e^{-1}$, respectively. All calculations were done using generalized gradient approximation (GGA) with parametrization (PBE) [21].

III. STRUCTURAL RELATIONS

In this section the main results for the structural properties of studied structures will be shown. To define optimal values of the lattice constants for each structure of $Zr - Nb$ alloy and structural relation c/a for the HCP crystals the optimization procedure was used.

A. BCC lattice

For alloys $Zr - xNb$ with BCC lattice the optimization procedure was made in the standard manner. For each value of Niobium concentration x we have defined the total energy for the unit cell of the crystal with varying

in the unit cell volume. Obtained data were approximated by the equation of state [22]. The minimum on the dependence of the total energy of unit cell versus unit cell volume corresponds to the optimal value of the unit cell volume. Following the standard definition for the volume of the unit cell of the BCC-crystals $V_{bcc} = a_{bcc}^3$ optimal value for the lattice constant a_{bcc} was defined. The dependence of the optimal lattice constant a_{bcc} on the Niobium concentration x for BCC alloys $Zr - xNb$ is shown in Fig.1.

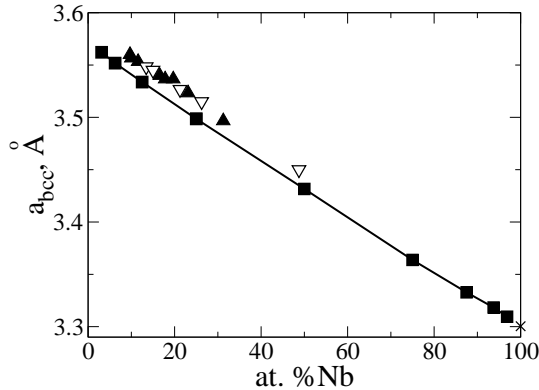


FIG. 1: Dependence of the lattice parameter a_{bcc} for the BCC alloys $Zr - Nb$ versus Niobium concentration.

Here, obtained theoretical results are shown with the help of filled squares. Empty and filled triangles correspond to the experimental data (see Refs. [23] and [14], respectively). The known value for the lattice constant of pure BCC Niobium is shown by symbol \times . From Fig.1 it is seen that with an increase in the Niobium concentration in the BCC alloy $Zr - xNb$ the lattice constant decreases according to the linear law. This result is consistent with the well known approximate empirical rule, called in metallurgy Vegard's law [24]. According to this rule at constant temperature a linear dependence between the crystal lattice parameter of an alloy and the concentrations of the constituent elements is realized. Thus for the studied BCC alloy Nb_xZr_{1-x} , where Zirconium atoms are substitutional ones in the BCC Niobium lattice, the relation between lattice parameters for the pure Zirconium and Niobium and its alloy is given as follows: $a_{ZrNb}^{bcc} = x \cdot a_{Nb}^{bcc} + (1 - x) \cdot a_{Zr}^{bcc}$. Here value for the lattice constant of pure BCC Niobium is known, $a_{Nb}^{bcc} = 3.3004 \text{ Å}$, whereas $a_{Zr}^{bcc} = 3.5634 \text{ Å}$ — fitting parameter (at low temperatures Zirconium is characterized by the HCP lattice).

It should be noted that in the interval of Niobium concentration x from 10% to 50% in the BCC alloy $Zr - xNb$ experimental data are slightly exceed obtained theoretical ones. It is natural, due to the theoretical calculations were performed at low (zero) temperature, while the presented experimental results obtained at evaluated temperatures [14, 23]. It was experimentally shown, that in the crystal $Zr - xNb$ at ($\sim 700K$) BCC phase is realized at evaluated and large values for the Niobium con-

centration, i.e. $at.\%Nb > 10\%$ [14, 23]. In Fig.1 we also show values for lattice constant of BCC alloy at small Niobium concentrations. In the next Section making an analysis of the total energy values of the crystals at low (zero) temperature we shall define the minimal value of the Niobium concentration in the alloy $Zr - xNb$, when crystal will characterize by BCC lattice.

B. HCP lattice

Now let us consider alloys $Zr - xNb$ with HCP lattice. The optimization procedure allowing to find optimal lattice constants a_{hcp} and c_{hcp} for such crystals is more difficult then in the previous case for BCC lattice. It is due to that for the HCP alloy one should define a global minimum of the total energy of a crystal as a function of both the volume of unit cell and the structural relation c/a . To this end we have proceeded in the following manner. For each value of Niobium concentration a test value of structural relation c/a was fixed. The standard optimization procedure, like in the case of BCC lattice was used to define the optimal volume of unit cell corresponding to the minimum of the total energy as a function of the unit cell volume, $E_{min}^{(i)}((c/a)_i)$, where $i = 1 \dots N$, N is a number of test values for the structural relation c/a . Obtained empiric data as dependence $E_{min}(c/a)$ were approximated by a functional dependence. Minimum of this dependence corresponds to the optimal value of the structural relation $(c/a)_{opt}$ for each studied value of Niobium concentration x in the HCP alloy $Zr - xNb$. Next, for defined $(c/a)_{opt}^{Nb}$ the standard optimization procedure was made to define a global minimum of the total energy and the optimal unit cell volume, respectively. Using the standard definition for the volume of the HCP unit cell $V_{hcp} = (c/a)_{opt} a_{hcp}^3 \sin(2\pi/3)$ the optimal lattice constant a_{hcp} was defined for each studied value of the Niobium concentration in the alloy. Obtained results for the lattice constant a_{hcp} and the structural relation c/a as functions on the Niobium concentration x in the HCP alloy $Zr - xNb$ are shown in Figs.2a and 2b, respectively.

In Figures 2a and 2b obtained theoretical results are shown by circles. By symbol \times values for the pure HCP Zirconium are shown. First, let us consider dependence of the lattice constant a_{hcp} versus Niobium concentration, shown in Fig.2a. It is seen, that increase in the Niobium concentration x in the HCP alloy $Zr - xNb$ leads to decrease in the lattice constant a_{hcp} , like in the case of the BCC crystals. However, in contrast to the previous case, the falling down dependence $a_{hcp}(at.\%Nb)$ differs from the linear for the shown interval of the Niobium concentration values. At low values of Niobium concentrations ($at.\%Nb < 20\%$) calculated data for the lattice constant a_{hcp} lie on the linear dependence, but for large $at.\%Nb$ one has deviation from the linear law. Thereby, empiric Vegard's rule for the studied HCP alloys can be applied in the case of low values of Niobium concentration x in al-

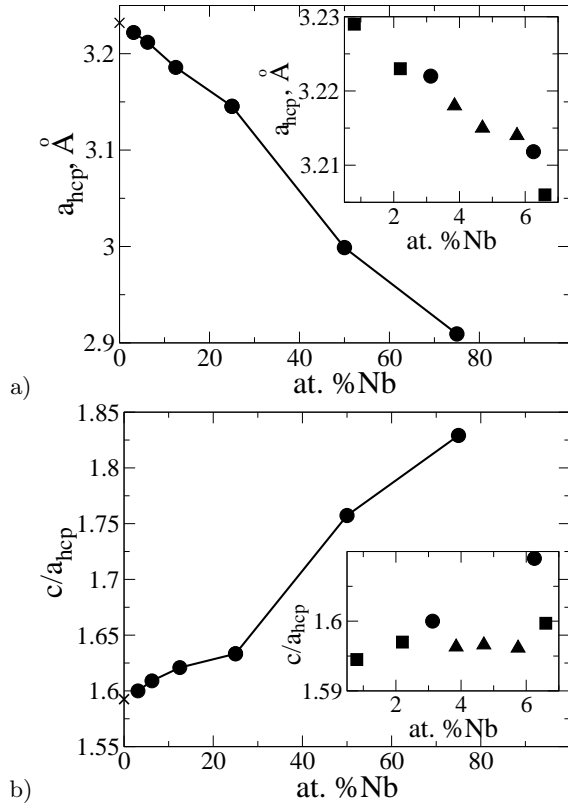


FIG. 2: Dependencies of the lattice parameter a_{hcp} (a) and structural relation c/a (b) for the HCP alloys $Zr-Nb$ versus Niobium concentration.

loys $Zr-xNb$. In the insertion in Fig.2a we have shown obtained theoretical results for a_{hcp} at low $at.\%Nb$ together with experimental data presented by triangles and squares from [14] and [25], respectively. One can see good quantitatively correspondence with experimental results for small values of Niobium concentration.

Next, let us consider dependence of the structural relation c/a as a function on the Niobium concentration x for the HCP alloys $Zr-xNb$ shown in Fig.2b. Here, marking is made in the same way, as in Fig.2a for the lattice constant. It is seen, that an increase in the Niobium concentration in the alloy leads to a grow of the structural relation c/a . It means, that the unit cell becomes more prolongate in z -direction. As for the lattice constant a_{hcp} for the structural relation c/a the falling down dependence versus Niobium concentration differs from the linear law; the last can be applied only for small values of $at.\%Nb$. Comparison of results obtained for HCP $Zr-Nb$ alloy with experimental data from Refs.[14, 25] for structural relation c/a at $at.\%Nb < 10\%$ gives small deviation, which is less than 1% (see insertion in Fig.2b).

Experimental investigations at $T \sim 700K$ indicate that HCP phase in $Zr-Nb$ alloys is realized only if $at.\%Nb < 6.5\%$ [14, 25]. Next, analyzing values of the total energy the maximal Niobium concentration value in alloy $Zr-Nb$, when alloy still characterizes by HCP lattice at low (zero) temperature will be defined.

IV. TOTAL ENERGY AND DENSITY OF STATES

Previously we have calculated optimal values for lattice constant for alloys $Zr-xNb$ with BCC and HCP lattices at different values of Niobium concentration x . Due to at normal conditions pure Zirconium characterized by the HCP lattice but pure Niobium has BCC lattice one can expect that at fixed temperature there is a critical value for Niobium concentration x_c corresponding to the structural transformation $HCP \rightarrow BCC$. It means, that for alloy $Zr-xNb$ at $x < x_c$ energetically more favorable will be HCP structure, whereas at $x > x_c$ BCC structure will be realized. Experimental investigations of Zirconium-Niobium alloys at high temperatures ($T \sim 700K$) show that in such conditions the critical Niobium concentration lies in the interval from 7 to 10 % [14, 23, 25].

To define the critical value of the Niobium concentration x_c at low (zero) temperature we shall analyze the total energies of all studied crystals with both HCP and BCC lattices and determine the energetically most favorable structure (HCP or BCC) for each model. To that end we proceed in the following manner. For fixed Niobium concentration x using obtained optimal lattice constant a_{bcc} , a_{hcp} and, in the case of HCP lattice, structure relation c/a we make a full cycle of *ab-initio* calculations to define the total energy for the unit cell. The unit cell contains 32 atoms for each structure due to the maximal number of atoms (32) in the unit cell have structures $Zr-3.125\%Nb$ (1 atom of Niobium and 31 atoms of Zirconium) and $Zr-96.875\%Nb$ (31 atoms of Niobium and 1 atom of Zirconium). Next, we define the difference between total energies for the unit cell of 32 atoms of HCP and BCC lattice, as:

$$\Delta E_{tot}(at.\%Nb) = E_{tot}^{uc}(at.\%Nb)|_{hcp} - E_{tot}^{uc}(at.\%Nb)|_{bcc}.$$

Hence, the value $\Delta E_{tot}(at.\%Nb)$ defines the type of energetically most favorable lattice for the alloy $Zr-xNb$ at fixed value of Niobium concentration x as follows: (i) if $E_{tot}^{uc}(at.\%Nb)|_{hcp} < E_{tot}^{uc}(at.\%Nb)|_{bcc}$, and as a result $\Delta E_{tot}(at.\%Nb) < 0$, then alloy $Zr-xNb$ has HCP lattice; (ii) at $E_{tot}^{uc}(at.\%Nb)|_{hcp} > E_{tot}^{uc}(at.\%Nb)|_{bcc}$, that gives $\Delta E_{tot}(at.\%Nb) > 0$, the BCC lattice is realized. Therefore, the critical value of the Niobium concentration x_c (or $(at.\%Nb)_c$) that defines the structural transformation $HCP \rightarrow BCC$ at fixed temperature (low/zero temperature in the studied case) can be defined from the condition of energetic equivalence of two lattices, i.e. $\Delta E_{tot}(at.\%Nb) = 0$. Obtained results for the difference of the total energies of the unit cell of 32 atoms versus Niobium concentration in alloy $Zr-Nb$ are shown in Fig.3.

It is seen that ΔE_{tot} changes a sign from minus to plus in the vicinity of the critical value of Niobium concentration $(at.\%Nb)_c \simeq 20\%$. Therefore, at low (zero) temperature the alloy $Zr-Nb$ with the Niobium concentration less than 20% is characterize by the HCP lattice

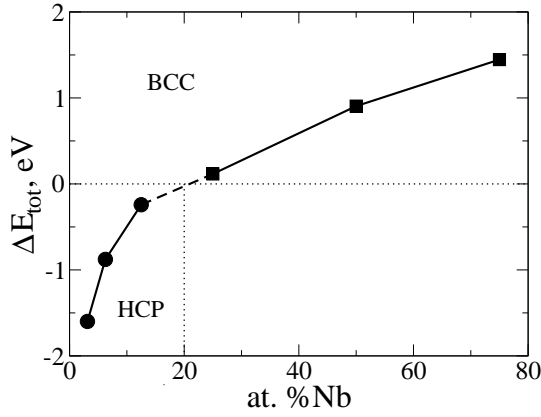


FIG. 3: A difference in the total energy of HCP and BCC structures $\Delta E_{tot}(at.\%Nb)$ in eV for the unit cell of 32 atoms as a function of the Niobium concentration in percents for alloys $Zr - Nb$.

($\Delta E_{tot} < 0$); values for the difference ΔE_{tot} are shown by circles. In the case of large Niobium concentration, more than 20%, the Zirconium-Niobium alloy has BCC lattice (squares in the Fig.3). Obtained result gives an explanation about the deviation from the linear dependence of the obtained results for the lattice constant a_{hcp} of the HCP alloys versus Niobium concentration for large $at.\%Nb$ (see Fig.2a).

As was pointed out before, experimental investigations for the Zirconium-Niobium alloys at high temperatures ($\sim 700K$) show, that the BCC phase is realized if $at.\%Nb \gtrsim 10\%$, whereas the HCP phase can be observed if $at.\%Nb \lesssim 6.5\%$ [14, 23, 25]. Thus, theoretically obtained result from *ab-initio* calculation for the critical value of Niobium concentration in the $Zr - Nb$ alloy ($at.\%Nb)_c \simeq 20\%$, that corresponds to the structural transformation $HCP \rightarrow BCC$ is about twice of the experimental one. An increase of the critical value of the Niobium concentration with a decrease in the temperature seems to be natural. With the temperature increase one gets that thermal fluctuations become large in the vicinity of the lattice knots. It leads to the destruction of the more complex HCP structure at smaller Niobium concentration. Hence one can expect a falling down dependence of the critical Niobium concentration ($at.\%Nb)_c$ in alloy $Zr - Nb$ versus temperature.

As far as obtained critical Niobium concentration at low (zero) temperature is ($at.\%Nb)_c \simeq 20\%$, next we perform calculations of the density of states (DOS) for two structures: $Zr - 12.5\%Nb$ and $Zr - 25\%Nb$, which are characterized by different energetically more favorable lattices, HCP and BCC, respectively. Obtained results are shown in Fig.4. Here, solid curves correspond to alloys with HCP lattices, whereas dash ones relate to alloys with BCC lattices. It is seen, that for the alloy $Zr - 12.5\%Nb$ the amplitude of the main peaks in the density of states is larger for the BCC lattice (see Fig.4a), whereas for the structure $Zr - 25\%Nb$ situation is quite

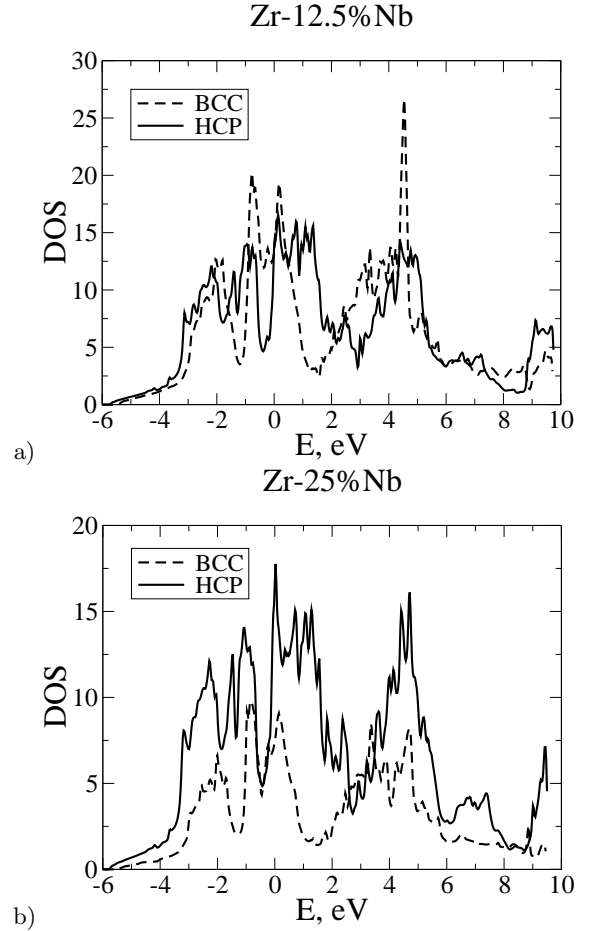


FIG. 4: Dependencies for densities of states (DOS) versus energy measured from the Fermi energy for: (a) alloy $Zr - 12.5\%Nb$; (b) alloy $Zr - 25\%Nb$ in the case of HCP lattice (solid curves) and BCC lattice (dash curves).

different: larger DOS corresponds to the alloy with HCP lattice (see Fig.4b). These results confirm that at low (zero) temperature alloy $Zr - 12.5\%Nb$ is characterized by the HCP lattice, whereas alloy $Zr - 25\%Nb$ has BCC lattice.

V. CONCLUSIONS

We have studied structural properties of the Zirconium-Niobium alloys with different Niobium concentrations in the framework of *ab-initio* calculation, using the density functional theory (DFT), linearized augmented plane wave (LAPW) method and generalized gradient approximation (GGA) with parametrization (PBE) at low (zero) temperature. Niobium concentration was varied from 3.125% to 96.875%. Models with BCC and HCP lattices for each considered Niobium concentration in alloy were studied. Using the optimization procedure to find a global minimum of the total energy of a crystal the optimal values for the lattice constants, and in

the case of HCP lattice, structural relation c/a were obtained.

We have found, that introduction of Zirconium atoms, as substitutional ones into the BCC crystal of Niobium leads to increase in the lattice constant. Obtained dependence of lattice constant versus Zirconium concentration in the BCC Niobium alloy is in good correspondence with empiric Vegard's law and is quantitatively consistent with known experimental data. Introduction of substitutional Niobium atoms into HCP Zirconium crystal

results to the decrease in the lattice constant and as a result to the increase in the structural relation c/a . The correspondence with the Vegard law, here, is realized only at small Niobium concentration (less than 20%), whereas obtained results are consistent with experimental ones. We have defined that at low (zero) temperature the critical value of the Niobium concentration in alloy $Zr-Nb$, which defines the structural transformation $HCP \rightarrow BCC$ is $(at.\%Nb)_c \simeq 20\%$.

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